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Quantum Computation for Physical Modeling

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1 Objectives

The objective of this task is to explore quantum computational models of dynamical physical systems. Focus is placed on compatible quantum computing algorithms, physical implementations, and architectures to simulate difficult physical systems that cannot readily be done by strictly classical means. Furthermore, the objective includes exploring approaches suited to a large array of small quantum computers.

2 Status of Effort

Natural quantum mechanical interactions in Carbon-13 have been controlled by nuclear magnetic resonance (NMR) to demonstrate simple quantum computations. The spin-1/2 nucleus of a Carbon-13 isotope in a magnetic field (10 Tesla) is used as a two-level quantum system. The two states of the nucleus, the spin-up and down (aligned and anti-aligned), are used to embody a qubit. Several Carbon-13 nuclei in the organic amino acid alanine,

have been used as proof-of-concept. Naturally occurring quantum mechanical interactions among the isotopes in this molecule have been coaxed using NMR spectroscopy to do simple sequences of quantum gates (for example, the collision operator for a quantum lattice-gas automaton) [1]. Essentially error-free NMR bulk computation allows for accurate and nondestructive qubit measurement using a large ensemble ($\sim 10^{18}$) of identical quantum computers. Preliminary NMR gate sequences for modeling fluid mechanics (the continuity equation and the Navier-Stokes equation) are undergoing testing. Unfortunately, the present day NMR technique is not likely to scale to more than a dozen qubits per quantum computer and we have found it quite difficult to embodying large arrays of small quantum computers. Applying quantum computation to physical modeling requires lattice-based quantum computers with at least millions of nodes. Other promising approaches to quantum computing based on quantum dots, Josephson junctions, SQUIDs, spin electronics, optical lattices, and improved NMR spectroscopic techniques are therefore under consideration.

3 Accomplishments

Fundamental to all approaches is the computing algorithm. Their implementation and application impose trade-off conditions for algorithm complexity and the number of quantum computer elements. I have defined the following two types of quantum computing architectures: type-I quantum computers have global phase-coherence, and type-II quantum computers have local phase-coherence, limited both in space and time. In a type-I computer, each qubit may be entangled with any or all other qubits and the system wavefunction is phase coherent for the duration of the entire quantum gate sequence needed to implement a particular algorithm. The outcome may be determined by measuring one or a few qubits. Type-I quantum computers may be used, for example, for Shor’s factoring algorithm or a quantum lattice-gas algorithm for the many-body Schrödinger equation.¹ A type-II quantum computer represents a network or array of small quantum computers interconnected by classical communication channels. Each qubit may be entangled with only nearby qubits at a particular node of the quantum computer and for only for a short time. The system wavefunction is always

¹ A *quantum lattice gas* is a quantum spin system that mimics the behavior of a system of massive quantum particles, propagating and colliding on a discrete space-time lattice.

factorized into a tensor product state over the nodes. The outcome is determined by measuring qubits on all nodes of the array. Qubits spatially arranged in a regular periodic lattice and small groups of neighboring qubits are homogeneously updated by local quantum gate operations applied simultaneously across the lattice. Type-II quantum computer may be used, for example, for the quantum lattice-gas algorithm for Navier-Stokes fluid simulation [1]. The type-I approach initially appeared as the most promising, and has received almost exclusive attention. However, since its development may take decades, we have also focused attention on quantum algorithms suited to type-II architectures.

This year we tested whether a phase-coherent type-I quantum computer can be used to simulate quantum lattice gas for fluid dynamics simulation [2]. Using principles and concepts from quantum mechanics instead of from classical mechanics, we formulate “local collision rules” for an artificial microscopic particle dynamics.

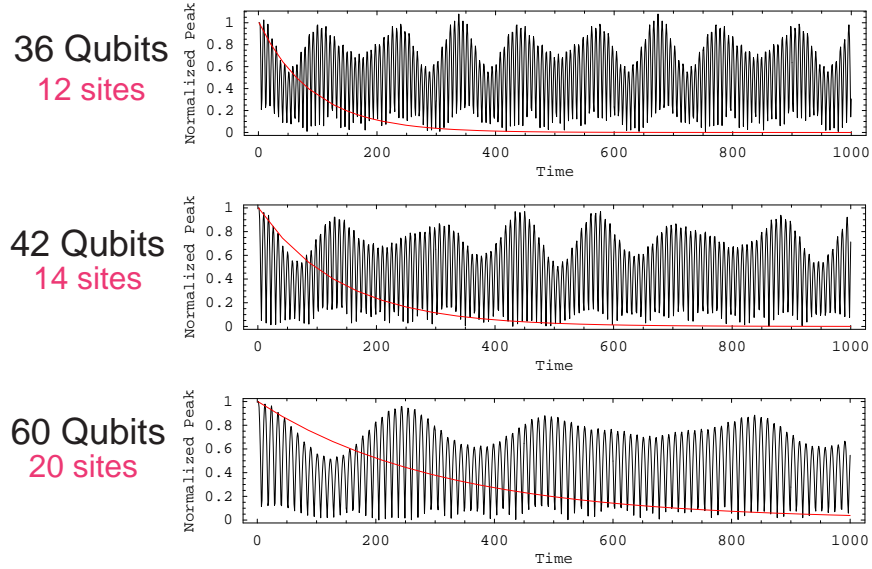


Figure 1: Oscillations of a mass density waves in the one dimensional quantum lattice gas for a system size of $V = 12, 14, 20\ell$ in the $m = 4$ and $p_x = 0 mc$ sector. The ordinate is the absolute value of the amplitude of the mass-density wave divided by the peak amplitude of the initial perturbation.

Numerical data taken from an exact simulation of a globally phase-coherent

quantum lattice-gas system was carried out for several systems with various grid sizes. The simulation method uses symbolic mathematics to implement a quantum mechanical system in the second quantized representation. A globally phase-coherent wavefunction is simulated on a classical computer. This is possible because the number of spatial sites of the lattice is relatively small (~ 60) and the number of qubits per site is few.² The main finding from the simulation is that viscous damping, as occurs in a classical fluid, is not observed in the one-dimensional quantum lattice-gas model. Instead, mass density waves oscillate indefinitely and the simulation confirms that there is both growth and damping in the hydrodynamic sound mode of the artificial fluid.

A time series history of the square of the peak amplitude is plotted in Figure 1 with three grid sizes and initial condition. In the quantum simulation, the peak amplitude does not decay in time, unlike the results obtained in the classical lattice-Boltzmann simulations. Initially, within the first couple dozen time steps, the peak amplitude begins to decay, very much like it does in a classical microscopic simulation or lattice-Boltzmann simulation of the model. However, the amplitude does not continue to damp in subsequent time steps. The peak amplitude rises and falls in a random fashion. No damping is observed even after a thousand time steps. Since the quantum algorithm is unitary (and hence the collisions obey the principle of detailed balance) the dynamics is reversible even though it is chaotic.

To obtain an accurate estimate of the sound speed of the mass density waves in the 1D quantum lattice-gas simulations, a Fourier transform of the time series history of the mass density at a single site of the system was computed and the power spectrum $\rho_\omega^*(x)\rho_\omega(x)$ plotted (see Figure 2). The signal, which is $\rho(6\ell, t)$, is measured at site $x = 6\ell$. Plotted is the power spectrum of the Fourier transform of the signal, which is $|\rho_\omega|^2$, versus sound speed (this is proportional to the oscillation frequency, $c_s = \ell f$). A peak in the power spectrum occurs just below the mean-field approximation of sound speed, which is plotted as the red vertical bar, but otherwise the simulation

²Since the numerical simulation is an exact treatment of a quantum spin system with 60 spins, this is actually a rather large computational task for a classical computer. Furthermore, since the size of the Hilbert space grows as 2^Q where Q is the number of spins (or qubits), it is not possible to store all the quantum basis states in memory at any one time. Fortunately, only a relatively small sector of the Hilbert space needs to be loaded into memory at any one time in our implementation of the quantum lattice-gas algorithm, which nevertheless uses an exact unitary evolution operator.

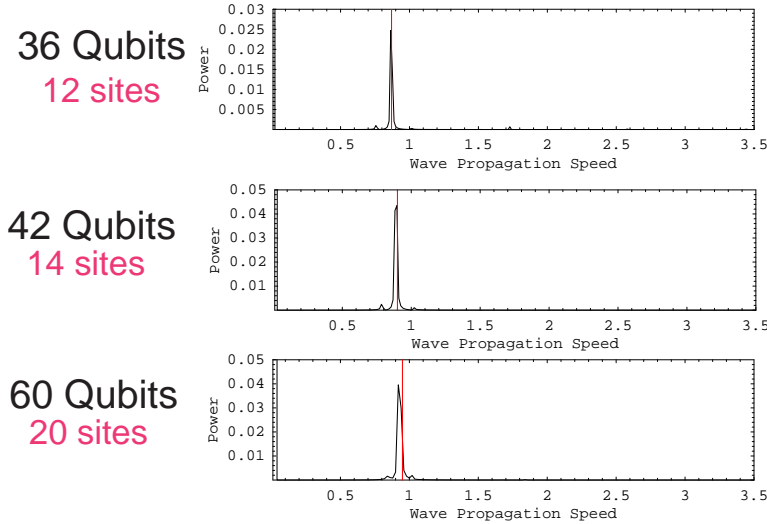


Figure 2: Discrete Fourier transforms of the time series data are taken to give $\rho_\omega^*(x)\rho_\omega(x)$. A peak in the power spectrum, $|\rho_\omega|^2$, occurs close to the predicted sound speed, which is plotted as the red vertical line. The abscissa is converted into unit of velocity, $c = \frac{\ell}{\tau}$, to show that there is a unique sound speed. The ordinate has units of $(\frac{m}{\ell} \times \tau)^2$.

and analytical results are in excellent agreement.

4 Personnel Supported

This fiscal year there were several researchers supported under the 2304TD task: Dr Bruce Boghosian, of the Boston U. Center for Comp. Sci., Dr Richard Nelson, of the MIT Francis Bitter Magnet Lab, and Harris Gilliam, of the Radex Corp. IPA agreements with Boston U. and MIT are used.

5 Interactions/Transitions

We are in close collaboration with MIT Nuclear Engineering Department for the purpose of building prototype quantum computer arrays using NMR spectroscopy. We are using specialized NMR spectrometers from Bruker Instruments Inc., NMR Division, Billerica, Massachusetts, with tightly coupled feedback and control system for producing very high accuracy scanning gra-

dient fields for spatial localization, addressing, and control, which is tailored to our needs.

6 Related Lectures

- *Invited Lecture* Cool Lessons in Science and Technology, “A Talk on Quantum Computation”, Air Force Research Laboratory, Hanscom AFB & Kirtland AFB 31 Mar 2000
- *Invited Lecture* Quantum Computing Colloquium, “Mesoscopic Quantum Computers for Physical Simulation”, Massachusetts Institute of Technology, Cambridge, Massachusetts 27 Sep 1999
- *Invited Lecture* 1st NASA International Conference on Quantum Computing and Quantum Communication, “Quantum Computers for Fluid Simulations”, NASA/JPL, Palm Springs, California 17 Feb 1998
- *Invited Lecture* MIT Media Lab, “Quantum Computers For Fluid Dynamics Simulation”, MIT E15-054, Massachusetts Institute of Technology, Cambridge, Massachusetts 22 Jan 1998

References

- [1] Jeffrey Yepez. Quantum computation of fluid dynamics. In Collin P. Williams, editor, *Quantum Computing and Quantum Communications*, page 480pp. Lecture Notes in Computer Science, Springer-Verlag, 1999. First NASA International Conference, QCQC’98, Palm Springs, California, USA, February 17-20, 1998, Selected Papers.
- [2] Jeffrey Yepez. A quantum lattice-gas model for computational fluid dynamics. *Physical Review E*, pages 1–45, Accepted 2000. APS E-Print: [aps1999Oct22_002](#).